



The next generation of Scientific Computing @AS

AFAD 2023

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Manager – Scientific Computing

Science. Ingenuity. Sustainability.

Who we are



Scientific Computing founded in June 2017



Support Science and Users

- Experiment Control
- Data Acquisition
- Data Processing
- Data Analysis



Our Team

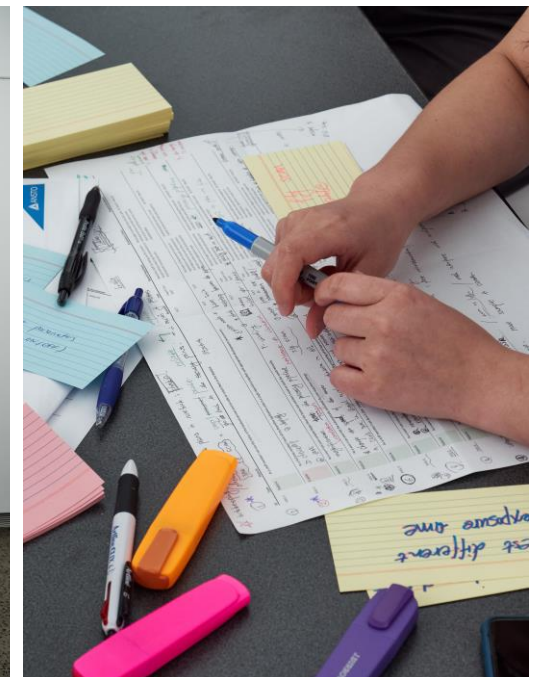
- 1 manager
- 20 members
 - 1 principal engineer
 - 2 DevOps
 - 10 PhDs
 - 50% gender split



Australian Synchrotron
Clayton, Victoria



User Stories



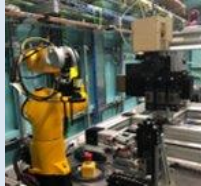
Australian Synchrotron & BRIGHT

A user focused facility

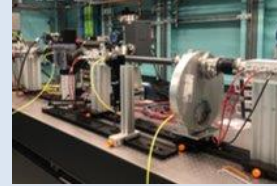
- 5500+ visits per year
- 10 (+2) operating beamlines
- 586 Journal Publications in 2022
- Generate 1.5 PB of data each year

A growing facility (BRIGHT program)

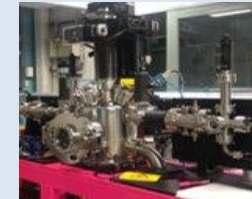
- 8 new beamlines
- 2 already operating
- Visits and data size going to double
- Opportunity to “refresh” software



Micro-CT
(8 – 40 keV)
Sept 2022



MEX-1
(3.5 - 13.6 keV)
Nov 2022



MEX-2
(1.3 - 3.5 keV)
Mid-2023



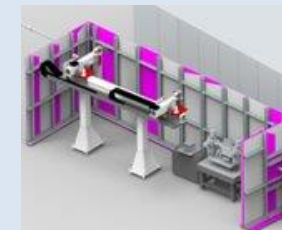
BioSAXS
(8 – 15 keV)
Mid-2023



MX3
(10-15 keV)
Mid-2024



ADS-1
(50 – 150 keV)
Late-2024

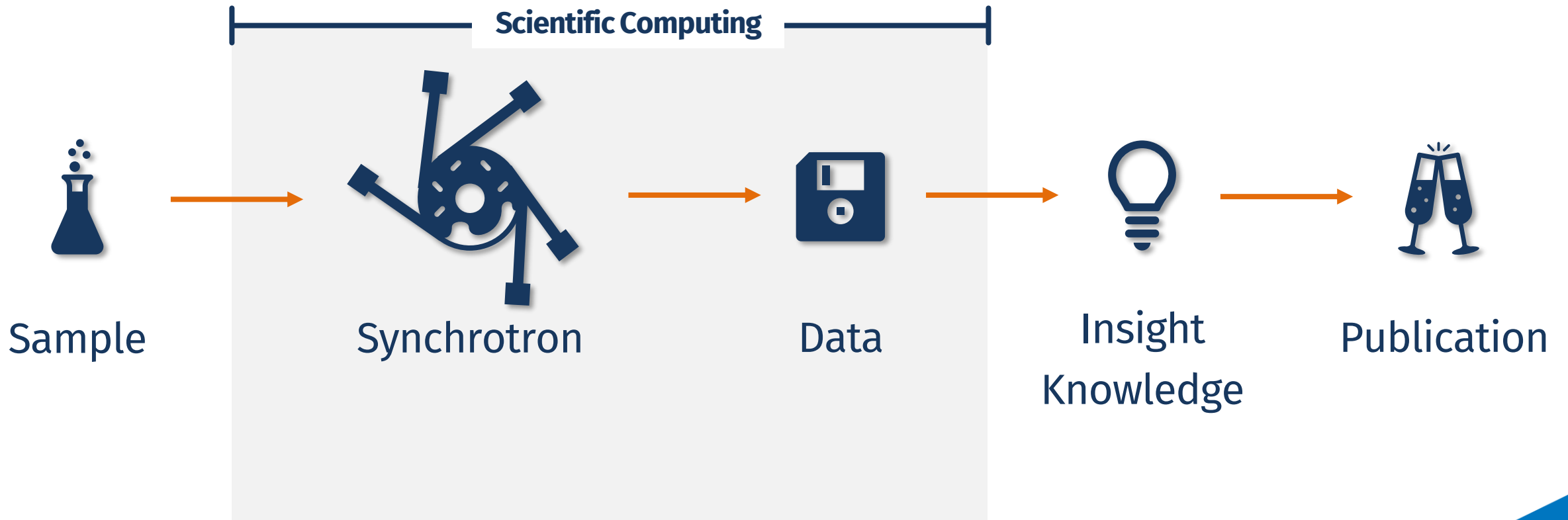


ADS-2
(45 – 90 keV)
Late-2024



NANO
(5 – 18 keV)
Mid-2025

A typical User Journey



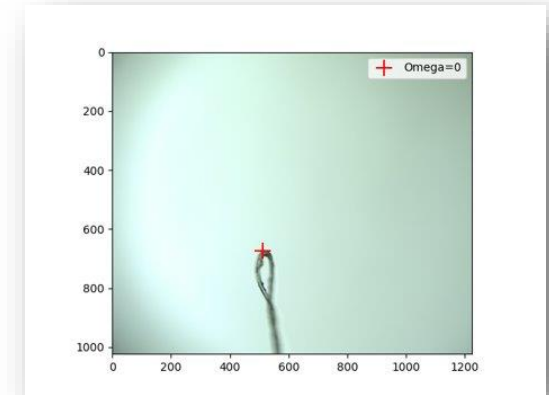
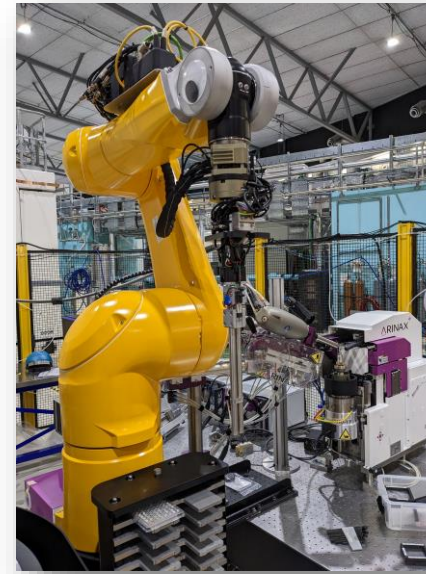
Samples & Robots

High throughput

- Robots loading samples
- Large number of samples
- Samples organised in trays, pucks, ...
- Connect samples to processing results

User friendly and fast

- Modern, web-based sample management applications
- Efficient sample changes
- Automated sample screening and quality checks



Home / Rebel Distributors Corp / Sending Trays

Sending trays from Rebel Distributors Corp

Tray ID

321 - SUPER-PROTEIN

	1	2	3	4	5	6	7	8	9	10	11	12
A	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
B	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
C	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
D	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
E	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
F	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
G	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
H	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Select wells to shoot by clicking wells or enter list separated by commas

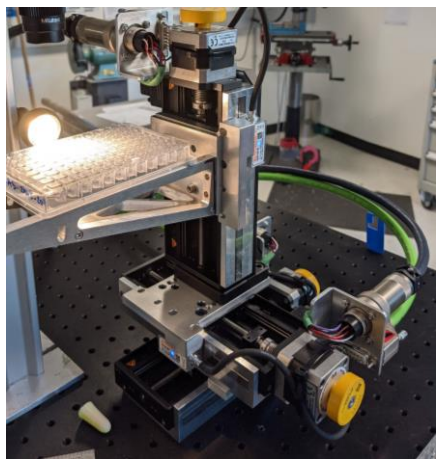
A9-1, A9-2, B9-1, B9-2, C9-1, C9-2, D9-1, D9-2, E9-1, E9-2, F9-1, F9-2, G9-1, G9-2, H9-1, H9-2, A4-1, A4-2, B4-1, B4-2, C4-1, C4-2, D4-1, D4-2, E4-1, E4-2, F4-1, F4-2, G4-1, G4-2, H4-1, H4-2, E8-2

Add another tray by entering ID in the top bar



Data Collection

Hardware



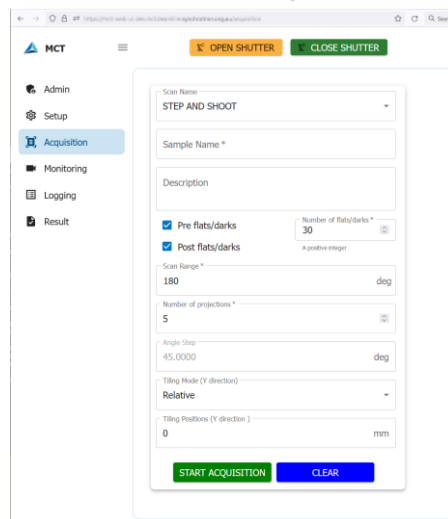
```
multi_2d_imaging.pyb
[6]: import os
# using ZMQ directly
from bluesky_queueserver_api.zmq import REManagerAPI
RM = REManagerAPI(zmq_control_addr=os.environ["BLUESKY_QUEUESERVE
RM.user = "root"
RM.user_group = "primary"
if RM.status()["worker_environment_exists"] != True:
    RM.environment_open()
    RM.wait_for_idle()

[7]: # Construct filename
filename = f"/data/{sample_name}.h5"

# Create a plan generator
generator = MCTPlanGenerator()

# Set plan values
generator.filename = filename
generator.description = description
generator.energy = energy
generator.detector_z_position = detector_z_position
generator.num_sample_images = num_sample_images
generator.num_flat_dark_images = num_flats_and_darks
generator.flat_stage_motor = flat_stage_motor
generator.flat_out_pos = out_pos
generator.flat_positioning_mode = flat_positioning_mode
generator.pre_darks = True
generator.pre_flats = True
generator.post_flats = True
generator.post_darks = True
generator.exposure_time = exposure_time
generator.sample_acquire_period = sample_acquire_period
generator.sample_y_positions = sample_y_positions

# Execute generated multi-2d plan
RM.item_execute(generator.multi_2d_aquisition_plan_dict())
RM.wait_for_idle()
```



Data Collection



Local Storage



Flexible experiment control

- Ophyd and Bluesky
 - Python abstraction layer and orchestration
 - developed by NSLS-II
 - sits on top of EPICS
- Controlled via
 - Web GUI for “normal” users
 - Jupyter notebook for “expert” user

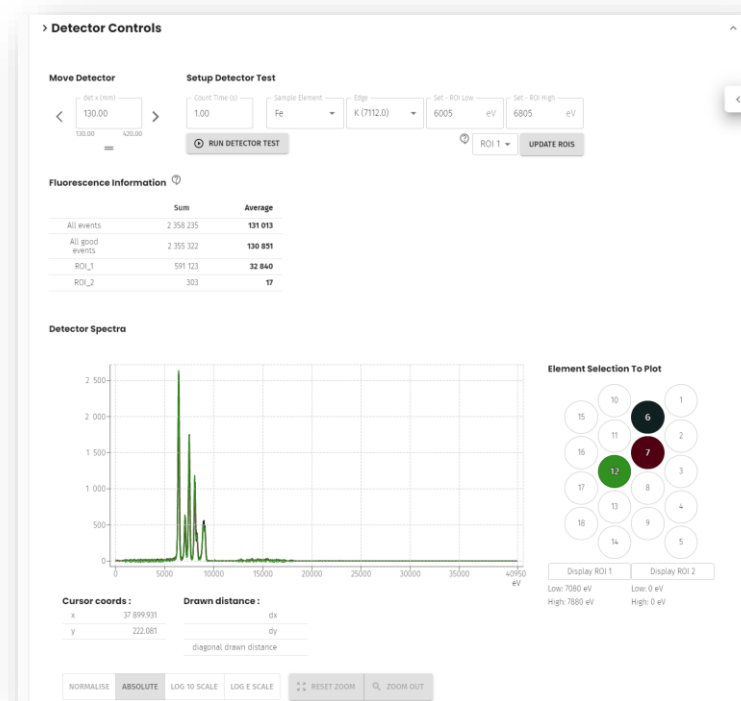
High throughput

- Stream data (avoid disk if possible)
- Capture rich metadata
- Store as “data product”

Web GUI

Modern interfaces

- Web-based GUIs
 - No local installation required
 - Remote access ready
- Established design language
 - Material UI
 - Reduces training time for users



	Gain	Counts	CPS
i0	10 ⁻⁵	2 815 175	2 815 175
i1	10 ⁻⁶	10 136 162	10 136 162
i2	10 ⁻⁷	6 450 848	6 450 848

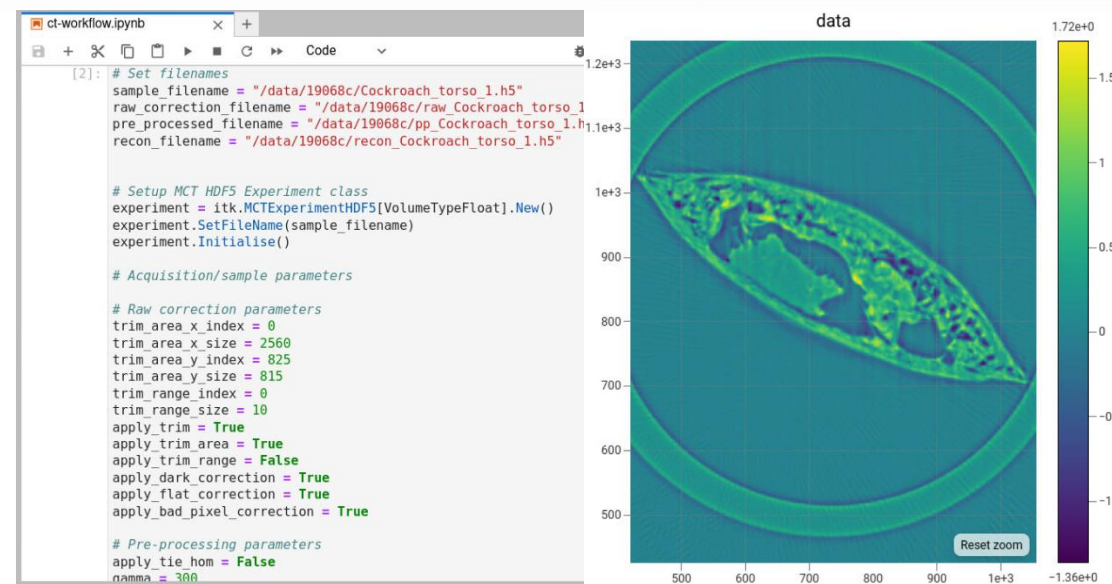
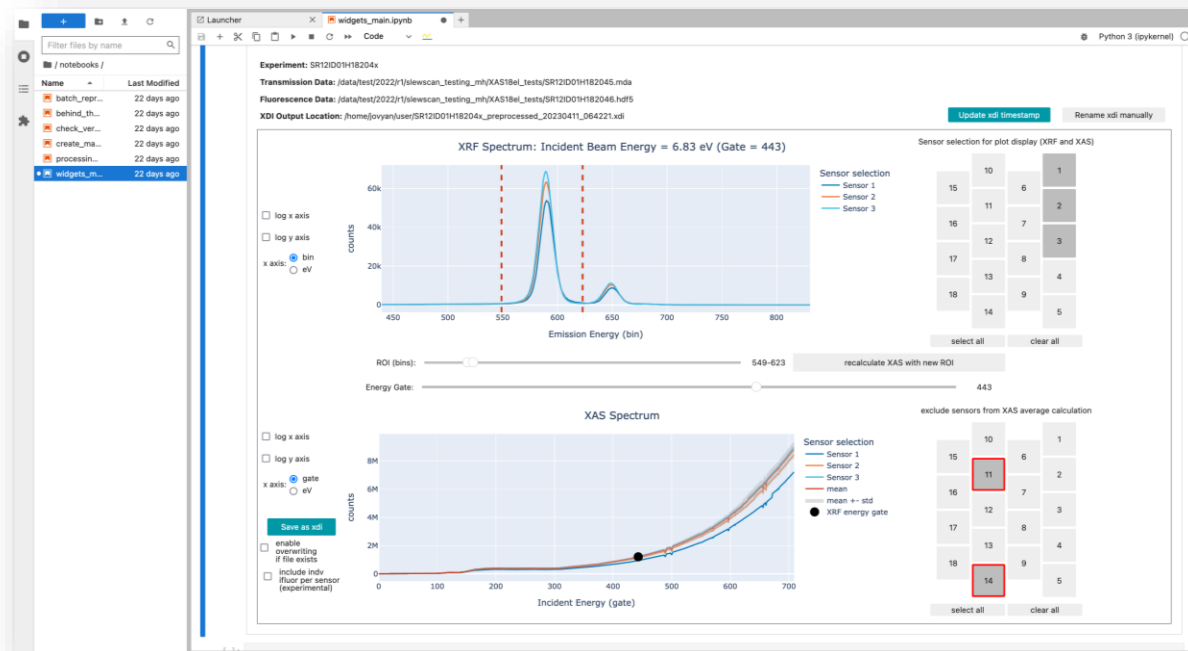
Positioner settle time: 0.30 | Detector delay time: 0.00 | Number of points: 815.00

Before Scan: Wait: 0.00 | After Scan: MEXIAUTOROCK:RUN.PR

Data Processing

High performance computing

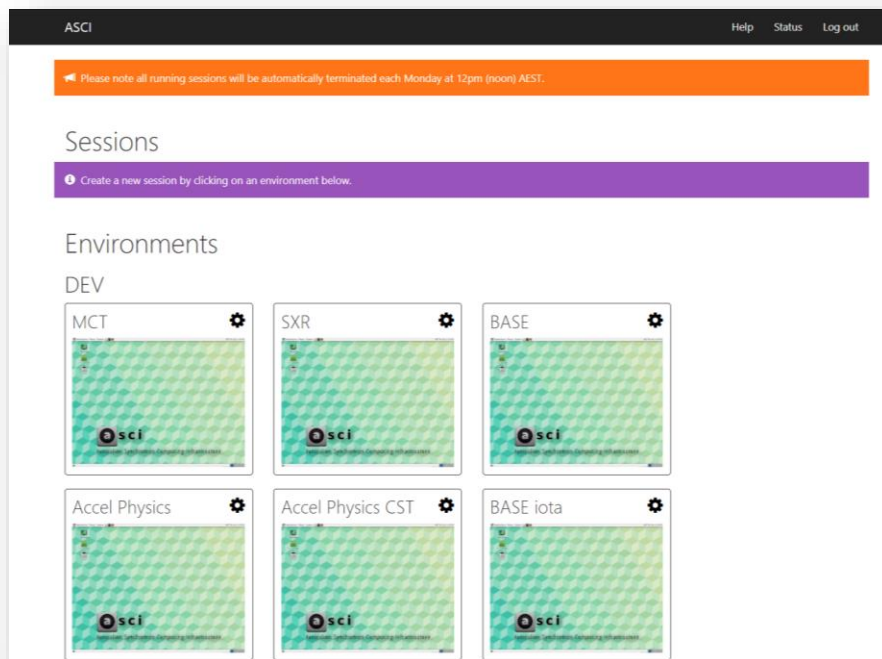
- HPC system
 - Comprised of 50+ physical servers
 - GPU nodes for image processing
- Beamline specific implementation
 - Heavily depends on beamline
 - Off-the-shelf and in-house tools
 - Heavy use of frameworks (e.g. ITK, Prefect)
 - Runs in Docker containers on Kubernetes



Data Analysis & Visualisation

Remote analysis platform

- Remote desktop environment in browser
- User starts session with tools pre-installed and data mounted



Data Management

We are only the temporary custodians of data

- Data has a lifecycle
 - Generated data is organised by datasets of “data products”
 - Our standard data container is HDF5
 - We delete data after 1 or 3 years (depends on beamline)
 - Space for 6PB locally
- Data transport
 - Users need to take their data home
 - We offer SFTP service
 - We will offer Globus in the future

From June 15th 2020, all data past its Policy Expiry Date will be deleted from our servers.

Australian Government | ANSTO [Data FAQ](#)

Data Records

EPN	BEAMLINE	TITLE	EXPIRY DATE
14412d1	SAXS	Understanding the roles of lipids in milk for oral delivery of drugs to combat infectious diseases: Part 3	19/03/2022
148692	SAXS	Understanding oligomisation of the human zinc transporter proteins	15/06/2020
1486923	SAXS	Understanding oligomisation of the human zinc transporter proteins	12/08/2026
14280d3	IMBL	Towards implementation of medical phase-contrast breast CT at IMBL. 3. Imaging full mastectomy samples with different types of breast cancer	19/03/2022
14280d4	IMBL	Towards implementation of medical phase-contrast breast CT at IMBL. 3. Imaging full mastectomy samples with different types of breast cancer	15/06/2020
14280d5	IMBL	Towards implementation of medical phase-contrast breast CT at IMBL. 3. Imaging full mastectomy samples with different types of breast cancer	15/05/2020



Infrastructure



Private cloud

■ DevOps & Containerisation

- Everything runs in a Docker container
- Fully automated CI/CD pipeline
- Dedicated DevOps engineer
- Infrastructure as Code
- No ssh'ing into VMs, no creation of snowflake machines

■ Industry standard orchestration

- All containers run in Kubernetes (including EPICS clients)
- Deployed through Helm charts
- Logging through ELK
 - › Currently investigating Sentry

The screenshot shows the Kubernetes dashboard interface. The main content area displays a table of Pods. The table has columns for Name, Images, Labels, Node, Status, Restarts, CPU Usage (cores), Memory Usage (bytes), and Created. The Pods listed include various components like proxy, hub, queue-server, and web-UI, all running on nodes in the 'beamline' namespace.

Name	Images	Labels	Node	Status	Restarts	CPU Usage (cores)	Memory Usage (bytes)	Created
mct-jupyterhub-proxy-56f848b4-9tw28	jupyterhub/configurable-http-proxy:4.5.3	component: proxy	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	3 hours ago
mct-jupyterhub-hub-8ff5bc55f-vp4cx	jupyterhub/hub:2.0.0	component: hub	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	3 hours ago
mct-bluesky-queue-server-prod-6589f8ccbb-muzht	docker.asci.synchronotron.org.au/mct/mct-bluesky-queue-server:1.4.22.3	app.kubernetes.io/instance: mct-bluesky-queue-server	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	3 hours ago
mct-bluesky-queue-server-stage-7c459cc4fb-rtfq	docker.asci.synchronotron.org.au/mct/mct-bluesky-queue-server:1.4.22.3	app.kubernetes.io/instance: mct-bluesky-queue-server	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	3 hours ago
mct-bluesky-queue-server-dev-76c7b745f-nr4x	docker.asci.synchronotron.org.au/mct/mct-bluesky-queue-server:main	app.kubernetes.io/instance: mct-bluesky-queue-server	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	3 hours ago
mct-acquisition-api-prod-565b9cd9f9-d4qct	docker.asci.synchronotron.org.au/mct/mct-acquisition-api:0.5.37-200	app.kubernetes.io/instance: mct-acquisition-api	vm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	4 hours ago
mct-web-ui-prod-d9999c8c-cr84s	docker.asci.synchronotron.org.au/mct/mct-web-ui:0.7.17-164	app.kubernetes.io/instance: mct-web-ui	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	5 hours ago
mct-web-ui-stage-6ddfc9c55-zndds	docker.asci.synchronotron.org.au/mct/mct-web-ui:0.7.17-164	app.kubernetes.io/instance: mct-web-ui	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	5 hours ago
mct-web-ui-dev-557c7486d9-c5tah	docker.asci.synchronotron.org.au/mct/mct-web-ui:main	app.kubernetes.io/instance: mct-web-ui	pm-01.nodes.imgnetes.beamline.synchronotron	Running	0	-	-	5 hours ago

